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Application of Photochemical Models Volume II. Applicability of Selected Models for Addressing Ozone Control Strategy Issues

Association of Bay Area Governments
Berkeley, CA

Prepared for

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Application of Photochemical Models

Volume II

Applicability of Selected Models for Addressing Ozone Control Strategy Issues

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APPLICATION OF PHOTOCHEMICAL MODELS

Volume II

Applicability of Selected Models for Addressing Ozone Control Strategy Issues

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PREFACE

This document is one of four volumes intended to provide information relevant to the application of photochemical models in the development of State Implementation Plans. The reports are particularly directed toward agencies and individuals responsible for preparation of non-attainment plans and SIP revisions for ozone. The four volumes are titled as follows:

Application of Photochemical Models

Volume I - The Use of Photochemical Models in Urban Ozone Studies

Volume II - Applicability of Selected Models for Addressing Ozone Control Strategy Issues

Volume III - Recent Sensitivity Tests and Other Applications of the LIRAQ Model

Volume IV - A Comparison of the SAI Airshed Model and the LIRAQ Model

This work is to a large extent based on the photochemical modeling experience gained in the San Francisco Bay Area in support of the 1979 Bay Area Air Quality Plan. The following individuals made significant contributions to this work:

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Bay Area Air Quality Management District	- Lewis H. Robinson - Rob E. DeMandel - Tom E. Perardi - Michael Y. Kim
Lawrence Livermore Laboratory	- William H. Duewer
Systems Applications, Inc.	- Steven D. Reynolds - Larry E. Reid

The authors wish to express their appreciation to John Summerhays, EPA Project Officer in the Source Receptor Analysis Branch of OAQPS, for his thoughtful review and comments on earlier drafts of this report.

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INTRODUCTION

BACKGROUND

Over the past several years a variety of photochemical models have been developed to describe the relationship between ozone precursor emissions and subsequent ozone production in the atmosphere. These model development efforts have been reviewed on numerous occasions. (See, for example, Systems Applications, Inc., 1976, U.S. EPA, 1977, and Argonne National Laboratory, 1977.) A primary objective in the development of these models has been to evaluate the effectiveness of alternative emission control strategies in reducing ambient ozone levels. At present, six ozone control strategy issues can be identified as being potentially significant for any region with an ozone problem. The purpose of this model assessment is to evaluate the applicability of selected models to the control strategy issues identified.

Since no quantitative, side-by-side comparison tests of ozone model performance have been made to date, judgments concerning the adequacy of treatment of a particular issue by a given model have been limited to aspects of the model's basic theoretical structure. For example, no judgment is made regarding the adequacy of a 31-step chemical kinetics mechanism versus a 51-step or 76-step mechanism--they all replicate smog chamber data and whether one is "more valid" than another is arguable at this point. Conversely, if a key variable is ignored or assumed to behave in a way which is known to be untrue under certain circumstances, then a judgment is made regarding the applicability of the model to such circumstances. The evaluation is presented on two levels: First, the general features and limitations of each type of modeling approach are reviewed with respect to the issues; and, second, more detailed aspects and applications of specific models are presented.

ALTERNATE APPROACHES TO OZONE MODELING

The variety of ozone models currently available may be categorized as rollback models, empirical models or deterministic models. Rollback models are the simplest, easiest and cheapest models available. While there are various forms of rollback models, they are all based on the presumption that for any given region a reduction in hydrocarbon emissions will produce a proportional reduction in maximum ozone levels. The complexities of the ozone formation and transport process are ignored, and the models are difficult in practice to validate due to lack of reliable historical emissions inventory and air quality data. Empirical models use existing air quality monitoring data and/or data from laboratory smog chamber studies to deduce the sensitivity of maximum ambient ozone concentrations to changes in ambient hydrocarbon and NOx concentrations. Theoretically, empirical models could, with the appropriate input data, be formulated to address any question of interest. Due to the practical limitations of existing data, however, application of existing empirical models to the evaluation of alternative control strategies requires an assumption that the ambient

hydrocarbon and NOx concentrations used are directly proportional to regional emissions for each pollutant. In addition, since monitoring data are used in the construction of the model, there is no simple means by which the model's performance can be evaluated.

Deterministic models attempt to mathematically describe the behavior of pollutants in the atmosphere. They may be further subdivided into three major classes: Gaussian, Lagrangian, and Eulerian. Gaussian models are relatively simple and presume both spatially uniform and steady-state atmospheric conditions. As a result they cannot be validly applied to describe the time-varying chemical and meteorological processes involved in ozone formation. Lagrangian models "trace" a parcel of air as it is carried by the wind across a given area. Typically, Lagrangian models focus on the chemistry of ozone formation within an "air parcel" while portraying meteorological transport and diffusion processes in simplistic terms. Finally, Eulerian models define a fixed grid over a given area. Pollutant mass is passed from one grid cell to another according to wind, diffusion, and chemical reaction parameters specified for each cell at each time step. Eulerian models are generally the most sophisticated, require the most input data, are the most expensive to run, and provide the most output information.

Because deterministic models are based on mathematical representations of physical and chemical processes, an evaluation of model performance is possible for a given region by comparing model simulations of historical conditions with the ozone levels recorded under those conditions. While such a comparison does not necessarily confirm a model's capability to predict future situations, it at least provides an intermediate point at which model performance may be independently assessed.

OZONE CONTROL STRATEGY ISSUES

Available models may be applied to six ozone control strategy issues. The general characteristics of the modeling approaches previously summarized lead to certain general conclusions regarding their applicability in each case. The control strategy issues identified for this evaluation are described below, as are general conclusions regarding model applicability in each case.

Hydrocarbon vs. NOx Control

Ever since the mechanism for photochemical ozone formation was first identified, it has been known that the primary ingredients were hydrocarbons, oxides of nitrogen, and sunlight. The most obvious targets for control are anthropogenic sources of hydrocarbons and NOx; however, the relative emission reduction that should be applied to each precursor to achieve the ozone standard in most regions has never been adequately estimated. Recent model application efforts have begun to address this problem, but results have yet to be adequately verified. Thus, the first issue of significance in ozone modeling is: can available models be applied to provide estimates of the degree of

hydrocarbon and NOx control required to achieve the ozone standard in a given region?

Most of the modeling approaches in some way account for the roles of hydrocarbons and NOx in ozone formation. The rollback models do not include NOx and therefore cannot assess the effect of changes in NOx emissions on ambient ozone levels.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

Many of the models currently available incorporate a role for NOx in ozone formation. This feature may or may not be sufficient to allow the same models to be applied to assess whether a given region will attain a short-term (e.g., 1-to 3- hour average) NO2 standard. The setting of such a standard is called for in the 1977 Clean Air Act Amendments if the medical and scientific data support the need for such a health-based standard. The question is: can existing models be applied to simultaneously assess attainment of both ozone and NO2 ambient air quality standards in a given region?

Since attainment of a short-term NO2 standard has not been an issue of concern in the past, none of the existing models has ever been applied to such a question; therefore, there is little or no experience to suggest whether existing models could successfully address the issue. On a theoretical basis, there is no reason why each of the modeling approaches could not be redirected to address the issue of attaining a short-term NO2 standard, with each approach retaining a set of advantages and disadvantages similar to those previously described. However, the atmospheric conditions which result in a buildup of high NO2 levels differ from those which result in high ozone levels. Previous studies of model performance have focused on ozone-episode days, and there is a need to carry out studies on NO2-episode days in order to assess model performance under such conditions (i.e., additional evaluation and/or field verification would be required before existing models could be accepted as satisfactorily addressing a short-term NO2 standard).

Control of Low-Level vs. Elevated Emissions

Elevated stacks have long been used to reduce the maximum ground-level concentrations of such primary pollutants as particulate matter and sulfur dioxide. Whether elevated emissions of hydrocarbons or nitrogen oxides have a lesser impact on ground-level ozone concentrations than low-level emissions has not been established. If there is a difference in effect, then this could alter the relative cost-effectiveness of emission control for elevated vs. low-level sources. The issue from a modeling perspective is: can existing models assess the relative effect of comparable emission reductions from elevated vs. low-level emissions in a given region?

For a model to distinguish the difference between low-level and elevated emissions it must have spatial resolution in the vertical dimension. In addition, the model should include some treatment of plume rise and

other small-scale influences on plume dispersion and chemistry. Rollback or empirical models, which deal with aggregated regional emission totals, cannot address this issue. While the Lagrangian and Eulerian models explicitly address spatial resolution in the horizontal dimensions, not all incorporate the vertical resolution which would allow them to address this issue. In addition, regardless of the theoretical possibilities, proper validation of any model for this purpose ideally would involve the collection of meteorological and air quality data at varying levels above the ground--existing ground-level monitoring data which is commonly collected would provide only partial verification of a model to address this issue.

Selective Control of Hydrocarbon Compounds

Laboratory (smog chamber) studies of oxidant formation have shown that different hydrocarbon compounds react at different rates and produce varying levels of maximum ozone. Early efforts at hydrocarbon control (e.g., Los Angeles' Rule 66) focused on those compounds which were known to be highly "reactive". More recent studies seem to indicate that while the rate of ozone production may differ, the cumulative ozone production potential of most hydrocarbon compounds is roughly the same (Dimitriades, 1977). The issue is: can existing models be applied to determine the viability of a strategy that would selectively control emissions of specific classes of hydrocarbon compounds to attain the ozone standard in a given region?

For a model to distinguish the effect of controlling different hydrocarbon compounds it must take separate account of each class of compounds of interest. Lagrangian and Eulerian models include a chemical kinetics mechanism that may incorporate from one to several classes of hydrocarbon species. An emission inventory developed for input to such a model must be disaggregated into the species classifications by which the model makes its computations. Thus, the selectivity in the types of species control which may be assessed by a given model is restricted by the definitions of the species classifications used in the model. For example, if a model treats only one class of hydrocarbon compounds in its computations (e.g., total hydrocarbons or non-methane hydrocarbons) then that model cannot distinguish the difference between a control program which would remove a given quantity of a "highly reactive" compound and one which would remove a similar quantity of a less-reactive compound.

Long-Range Transport

There is an ample body of evidence indicating that ozone and ozone precursors can be and are transported over long distances beyond conventional "air basin" boundaries. The impact of emissions in one region on ozone levels in another has been an issue of concern in many areas across the nation. For this evaluation the general issue is: can existing models be applied to assess long-range transport of ozone and its precursors? This issue can be divided into two related issues: (1) can existing models be applied to assess the effects of long-range transport of pollutants from "upwind" sources on ozone levels in a given

study area?; and (2) can existing models be applied to assess the influence of emissions in the study area on levels of ozone and precursors in other areas downwind?

The impact of ozone transported into a study area can be considered in all the models evaluated in this report. The version of rollback sanctioned by EPA considers transport by relating a city's emissions specifically to the city's contribution to its ozone problem. A similiar process is performed in using the standard version of EKMA. The other models consider transport as a direct input into the model. Thus the remainder of this report will focus on the impact of a study area on the pollutant transport downwind.

The issue of influence of a study area on transport long distances downwind is complicated by the lack of a precise definition of "long-range". From a modeling standpoint, long-range could be defined as that distance over which the validity of the assumptions inherent in existing models becomes questionable. This distance will vary depending on the particular atmospheric conditions being modeled and the model being used. Rollback and available empirical models do not incorporate spatial resolution at all, hence they cannot be applied to address this issue. Lagrangian models are limited by the distance over which their assumptions of no horizontal diffusion or wind shear are valid. Both Lagrangian and Eulerian models may be limited by how well their chemical kinetics can simulate what occurs under nighttime conditions.

In each of these cases, there is little or no experience as to whether models in their existing forms can validly simulate the processes that result in long-range transport of ozone and ozone precursors. While it is conceivable that Lagrangian and Eulerian models could be modified to provide results over longer transport distances than is currently the case, the validity of the application depends to a large extent on the particular transport mechanism of significance over a given area. For example, a commonly suggested mechanism for long range transport involves pollutants that become trapped in stable atmospheric layers aloft, are transported long distances, and that then are transported to the surface at a location far removed from the original source area. A mechanism of this complexity cannot be addressed by existing models without further data acquisition and performance evaluation.

In general, available models are intended for application to urban areas with horizontal distance scales of roughly 10 to 100 kilometers. If the particular transport mechanism of significance in a given area can be identified, and if monitoring data are available to characterize the "upwind" boundary conditions for the study area, then existing models could be applied to assess the impact of pollutants transported into a given region. In general, however, calculation of effects over distance scales significantly greater than 100 kilometers would be best addressed using a model specifically designed for such purposes. For example, EPA is currently funding the development of a mesoscale photochemical model to be applied to the Northeastern United States.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

The complex process of ozone formation varies in space and time. Differing spatial and temporal emission patterns within a given region could possibly produce different ozone levels. Thus the issue is: can existing ozone models account for and be applied to assess the effects of alternative spatial and temporal patterns of precursor emissions?

The model requirements to address this issue are self-evident; only existing Lagrangian and Eulerian models can be applied to assess the effects of spatial and temporal emission variations. Of these, Eulerian models provide a more comprehensive format for investigation of this issue, since both input and output data cover the entire modeling region rather than selected trajectories.

SPECIFIC MODEL ASSESSMENTS

This section contains brief descriptions of selected ozone models for which versions are currently in the public domain. In many cases the models undergo periodic update and modification, so it is advisable to check with the developer of a given model to obtain details of any recent changes. The descriptions presented below are based on current versions of the models.

The specific models reviewed are as follows:

- o Linear Rollback
- o EKMA, developed by EPA
- o City-specific EKMA using Ozone Isopleth Plotting Package (OZIPP) developed by EPA
- o Hanna ATDL, developed by Atmospheric Turbulence and Diffusion Laboratory, NOAA
- o ELSTAR, developed by Environmental Research and Technology, Inc.
- o TRACE, developed by Pacific Environmental Services, Inc.
- o LIRAQ, developed by the Lawrence Livermore Laboratory
- o SAI Urban Airshed Model, developed by Systems Applications, Inc.
- o IMPACT, developed by Science Applications, Inc.
- o MADCAP, developed by Science Applications, Inc.

This sampling of available ozone models is not intended to be all-inclusive; rather, it is intended to be representative of the most widely-applied or most generally-accessible models available at this time. There have been numerous attempts over the past several years to develop ozone models, and the previous reviews cited can be consulted for appropriate references. There may be other perfectly adequate models in existence or currently under development which were excluded from this assessment; conversely, inclusion of a particular model in this assessment does not necessarily constitute endorsement of its use for any specific application.

Each model description includes a brief history of the model's development and previous applications, basic approach, variables considered, input data requirements, computer requirements (based on actual operating experience) and references for further documentation. Following each description is a discussion of the model's applicability to each of the ozone control strategy issues previously discussed. The results of the evaluation are summarized in simplified form in Table 1. This table is intended to provide summary information which supplements the more detailed discussion to follow, and should not be interpreted as providing a relative "ranking" of the models listed.

TABLE 1. SUMMARY OF MODEL ASSESSMENTS

Model	Type of Model	Ozone Control Strategy Issues: HC vs. NO_x Control	Assessing Attainment of Ozone Standard vs. NO_2 Standard	Low Level vs. Elevated Emission Control	HC Reactivity Control	Long Range Transport	Spatial and Temporal Emissions Variation	Data Requirements	Costs	Output
Rollback	-	4	4	4	4	4	4	a	A	C
EKMA, standard	E/S	3	4	4	4	4	4	a	A	C
EKMA, city-specific (OZIPP)	LT	3	4	4	3	4	3	b	B	B
HANNA ATDL	Box	3	4	4	4	4	4	a	A	C
ELSTAR	LT	1	2	3	1	3	1	b	B	B
TRACE	LT	1	2	4	1	3	1	b	B	B
LIRAQ	EG	1	2	4	1	2	1	c	C	A
SAI Airshed	EG	1	2	1	1	2	1	c	C	A
IMPACT	EG	1	2	2	1	2	1	c	C	A
MADCAP	EG	1	2	2	1	2	1	c	C	A

Type of Model

- E/S - empirical/statistical
- LT - Lagrangian Trajectory
- EG - Eulerian Grid

Issue Ratings

1. Demonstrated applicability (previous verification performed)
2. Theoretically applicable, limited by data availability (i.e., no previous verification performed)
3. Theoretical limitations (applicable only in limited circumstances)
4. Not applicable

Data Requirements Ratings

- a aggregated emissions data, no meteorological data
- b spatially, temporally, and species disaggregated emissions data, meteorological data along trajectory corridors
- c spatially, temporally, and species disaggregated emissions data, meteorological data throughout urban study area

Cost Ratings

- A inexpensive (little or no computer requirement)
- B moderate cost (moderate computer requirement, cost per run ranges from $10 to $100)
- C expensive (substantial computer requirements, cost per run ranges from $100 to $1,000)

Output Ratings

- A extensive output produced (e.g., hourly concentration fields for entire modeling region)
- B moderate output produced (e.g., concentrations along specified trajectories within the modeling region)
- C limited output produced (e.g., percent emission reduction required, or expected ozone maximim)

ROLLBACK

MODEL FEATURES

Model Type

Statistical

Historical Data

The concept of regional emissions rollback (deNevers, 1975 and Roth, 1976) had been practiced for many years prior to its sanction for use in the preparation of State Implementation Plans mandated by the Clean Air Act of 1970. During the 1970s rollback was used extensively for this purpose (Cheng, 1975 and DeMandel, 1978); many variations of the rollback technique have been devised but only linear rollback with corrections for background and transport has been accepted by the EPA.

Description

In rollback models the emissions/air quality relationship is simplistically displayed on a two-dimensional graph as shown in Figure 1. Using one of these rollback curves and knowing the highest or second highest one-hour average oxidant measurement during a given year, one could infer the percentage control of hydrocarbon emissions needed to achieve the ozone standard.

The technical basis of these models suffers from major deficiencies. Among these are the following:

- The role of NOx emissions in the formation of ozone is ignored.
- Varying photochemical reactivities for different organic compounds are ignored.
- The air quality effect of control strategies which result in non-uniform emission reductions over a given region cannot be evaluated (i.e., emission reductions must be assumed to occur uniformly).

Spatial Resolution

Horizontal - none

Vertical - none

Temporal Resolution

None

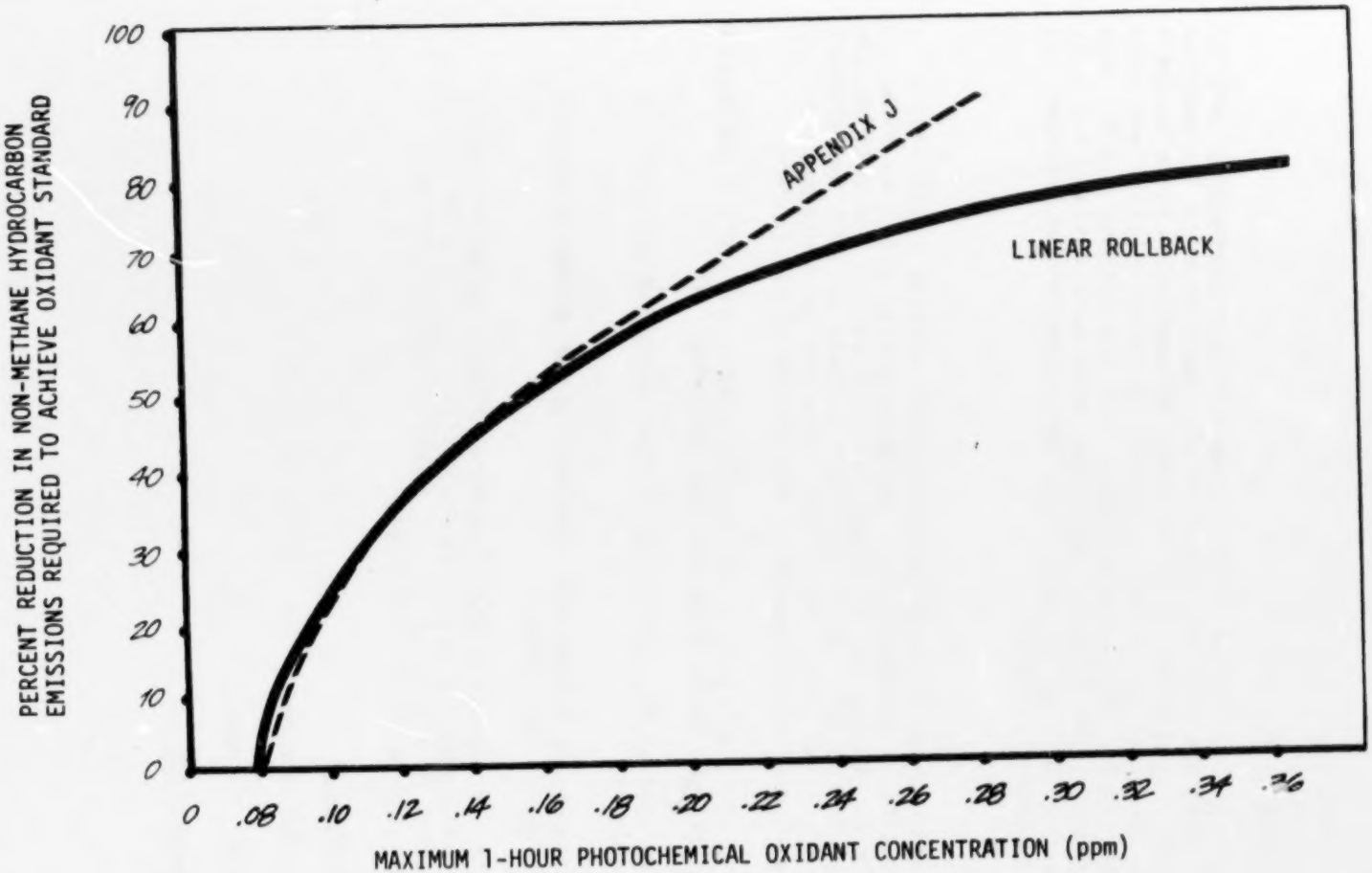

Figure 1. Comparison of Hydrocarbon Rollback Models

Meteorology

None

Chemistry

None

Input Data Requirements

Meteorological Variables - None

Emissions Data - annual, aggregated regional non-methane hydrocarbon inventory.

Air Quality Data - second highest ozone level in some selected base year.

Key Output

Percent reduction of regional non-methane hydrocarbon emissions required to achieve the ozone standard.

Approximate Computer Costs

No computer necessary.

APPLICABILITY OF ROLLBACK TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

Rollback techniques are not applicable to this issue because the role of NOx emissions in the formation of ozone is ignored.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

The principle of rollback can be applied to estimate the control requirements necessary to meet either an ozone standard via hydrocarbon emission reduction or an NO2 standard via reductions in NOx emissions. But because rollback does not acknowledge the chemical interaction of hydrocarbons and NOx, it cannot be used to weigh this issue.

Control of Low-Level vs Elevated Emissions

Rollback is applied to regionally aggregated emission inventories which are not defined by sources. It cannot be used to address this issue.

Selective Control of Hydrocarbon Compounds

The rollback technique does not make any provisions for various degrees of hydrocarbon reactivity and thus cannot be used to address this issue.

Long Range Transport

Rollback does not incorporate a transport mechanism and thus cannot be used to address this issue.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

Annual, regional emission inventories are used in rollback techniques. The model cannot be used to address this issue.

STANDARD EKMA (EMPIRICAL KINETIC MODELING APPROACH)

MODEL FEATURES

Model Type

Empirical

Historical Data

EKMA was released by EPA in November, 1977. Since then, several studies have been performed to compare EKMA results with other techniques (deNevers, 1978 and DeMandel, 1978) and numerous states have used the model in the development of their State Implementation Plans.

Description

EKMA was developed by the EPA as a more advanced ozone prediction relationship than ROLLBACK. EKMA is a series of isopleths that express the relationship between early morning downtown NOx and hydrocarbon levels and the peak ozone levels downwind of a city center under a given set of meteorological, emissions and air quality conditions (See Figure 2) (U.S. EPA, 1977). Theoretically, given a sufficiently large data base of observed early morning NOx and NMHC levels with the corresponding maximum afternoon ozone levels at a selected site and with a single meteorological scenario, a similar set of isopleths can be drawn for any site.

In EKMA, the reduction in a city's design ozone concentration caused by a given emissions reduction is assumed to be equal to the reduction that can be derived through the use of the plotted curves. This equality is assumed regardless of what conditions led to the city's design ozone concentration. A key output of EKMA is the effect of given HC and NOx emission reductions on expected maximum ozone levels.

For general applications, the EPA has developed a standard set of EKMA isopleths based on a predefined set of conditions (U.S. EPA, 1978). For more specific applications, a computer program is available to generate city-specific curves (U.S. EPA, 1978) which more closely match those conditions under which the design ozone concentration actually occurred. In both cases, the isopleths are derived using a kinetics model which is based essentially on a Lagrangian concept. The differences between a kinetics model and a Lagrangian model are 1) the formulations used to consider emissions and mixing height are different, and 2) the kinetics model is customarily applied with cruder assumptions than are used with Lagrangian models.

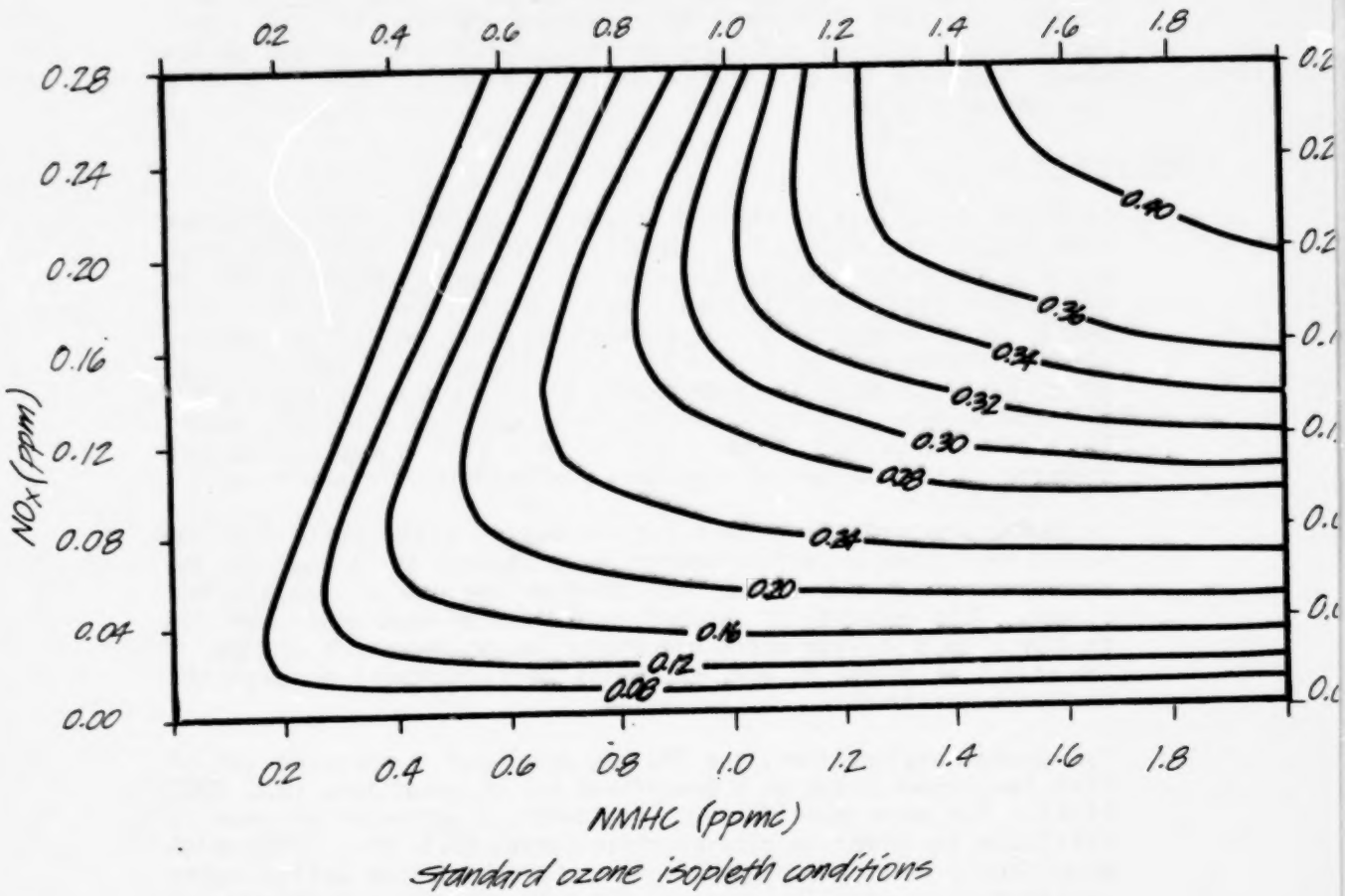

Figure 2. Example Standard EKMA Ozone Isopleth Diagram

Source: Environmental Protection Agency.
"Users Manual for Kinetics Model and
Ozone Isopleth Plotting Package,"
EPA-600/8-78-014a, July, 1978.

Spatial Resolution

Horizontal - none

Vertical - none

Temporal Resolution

None

Meteorology

None - A predefined meteorological scenario is assumed.

Chemistry

None - A predefined mix of hydrocarbon species and reactions is assumed.

Input Data Requirements

Meteorological Variables - none

Emissions Data - annual, aggregated non-methane hydrocarbon and NOx inventory.

Air Quality Data - second highest ozone level in some selected base year and the corresponding level of morning NMHC and NOx.

Key Output

Percent reduction of non-methane hydrocarbons and/or NOx to achieve the ozone standard.

Approximate Computer Costs

No computer necessary.

APPLICABILITY OF STANDARD EKMA MODEL TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

Because EKMA relates hydrocarbon and NOx levels to ozone concentrations, it can be used to address this issue. The isopleths are intended to be used to evaluate the effect of relative changes in regional non-methane hydrocarbon and NOx emissions on peak ozone levels. However, EKMA was not designed to predict absolute ozone values as a function of hydrocarbon and NOx levels and should not be thus applied.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

In theory EKMA can be used to generate a set of NO2 isopleths because a chemical kinetic mechanism is used to express the HC/NOx relationship. These isopleths could then be used to evaluate whether achieving an NO2 standard is counterproductive to reducing ozone levels or vice versa. The EPA is now developing a set of NO2 isopleths.

Control of Low-Level vs Elevated Emissions

EKMA employs a regionally-aggregated emissions inventory which does not distinguish between elevated and low-level sources. Therefore, the standard EKMA, cannot be used to address this issue.

Selective Control of Hydrocarbon Compounds

Because EKMA utilizes a predetermined mix of non-methane hydrocarbon compounds it cannot be used to address this issue.

Long-Range Transport

The standard EKMA isopleths are based on (and thus limited by) a ten-hour simulation along a hypothetical trajectory. The short simulation time is generally insufficient to treat long-range transport issues.

Effect of Spatial and Temporal Variation of Ozone Precursor Emissions

A predefined set of spatial and temporal emissions variations are assumed for EKMA standard method. Thus it is not applicable to this issue.

CITY-SPECIFIC EKMA USING OZIPP (OZONE ISOPLETH PLOTTING PACKAGE)

MODEL FEATURES

Model Type

Lagrangian Trajectory

Historical Data

See standard EKMA

Description

The city-specific EKMA (U.S. EPA, 1978) is patterned after a trajectory model. It is most applicable to cities with simple, uniform meteorology and emissions distribution, that can be characterized by a single trajectory. For this model, the trajectory is predetermined. With the city-specific EKMA it is possible to generate a set of ozone isopleths which more closely matches those conditions under which the design ozone concentration actually occurred.

Spatial Resolution

Horizontal - the precursor emissions can be apportioned along the predetermined trajectory path.

Vertical - none

Temporal Variation

Hourly precursor emissions are input to the city-specific EKMA. Peak ozone levels, because of the present meteorology, are assumed to occur in the early afternoon hours and are reported hourly.

Meteorology

A single scenario of a sunny day is assumed. A predetermined trajectory precludes the need for developing a wind field.

Chemistry

76-step reaction mechanism
three hydrocarbon classes: propylene, butane, and adehydes

Input Data Requirements

Meteorological Variables - mixing height, latitude, date.

Emissions Data - distribution of total precursor emissions along the trajectory on an hourly basis for NOx, NO2, propylene, butane, and aldehydes.

Air Quality Data - initial concentrations for all input species at the city center at the start of the simulation and for precursors and ozone along the trajectory.

Key Outputs

Set of isopleths showing the relationship between NOx and hydrocarbons for different resultant oxidant levels.

Approximate Computer Requirements

To generate a complete set of city specific isopleths (ten-hour simulations) requires seven minutes on a Univac 1110 along with 38K bytes of core. A single trajectory requires ten seconds of computation time.

APPLICABILITY OF THE CITY-SPECIFIC EKMA MODEL (OZIPP), TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

EKMA essentially attempts to relate the early morning precursor (hydrocarbons and NOx) concentrations to peak ozone concentration. Each precursor level can be adjusted independently of the other. Therefore, the city-specific EKMA can be used to address this issue.

The isopleths are designed to be used to evaluate the effect of relative changes in hydrocarbon and/or NOx emissions on the expected peak ozone levels. EKMA was not designed to estimate the absolute ozone values as a function of hydrocarbon and NOx levels and should not be thus applied.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

In theory EKMA can be used to generate a set of NO2 isopleths because a chemical kinetic mechanism is used to express the HC/NOx relationship. These isopleths would then be used to evaluate whether achieving an NO2 standard is counterproductive to reducing ozone levels or vice versa. The EPA is now developing a set of NO2 isopleths.

Control of Low-Level vs Elevated Emissions

The city-specific EKMA can not be used to address this issue. It is a single layer model and thus can not differentiate between emission sources at varying heights.

Selective Control of Hydrocarbon Compounds

Hydrocarbons are divided into three classes, propylene, butane, and aldehydes, and the amount of each emission can be varied to study their effect on ozone formation. Differences in the effectiveness of control programs directed at selected species within any one of these classes cannot be readily assessed.

Long-Range Transport

EKMA is limited to 10-hour simulations along a predetermined trajectory. Long-range transport implies multi-day simulation capabilities which EKMA does not possess. It is not capable of addressing this issue because it was not so designed.

Effect of Spatial and Temporal Variation of Ozone Precursor Emissions

The city-specific EKMA can be used to address the question of spatial and temporal variability along the trajectory path. The emissions input to the model are spatially resolved along the trajectory path and temporally resolved on an hourly basis.

HANNA ATDL PHOTOCHEMICAL MODEL (ATMOSPHERIC TURBULENCE AND DIFFUSION LABORATORY)

MODEL FEATURES

Model Type

Box

Historical Data

The Hanna ATDL model was released in 1973. No updates have been issued since. Model application has consisted of comparing its results against observations and predictions of more complex models.

Description

The ATDL is a stationary box model (Hanna, July, 1973 and Hanna, October, 1973). A volume of air is assumed to be the reaction vessel. Within this box, emissions are assumed to be mixed instantaneously. A gross representation of ventilation is simulated by a constant unidirectional wind. Fixed mixing heights are used for each stability classification. Concentrations of unreactive compounds are assumed to be directly proportional to each species' emission strength and inversely proportional to the wind, which is moving a quantity of pollutants out of the box per unit time.

To represent photochemical reactions, it is assumed that for any mechanism, a related set of dimensionless equations can be written relating the precursors and ozone levels. By analyzing the dimensionless quantities, the relative importance of the chemical reaction, meteorology and source strength to that species can be evaluated.

The ATDL technique of dimensionless equation analysis was applied to the five-equation photochemistry simulation developed by Friedlander and Seinfeld (Friedlander, 1969). This reaction mechanism consisted of three simple reactions for NO2, NO and reactive hydrocarbons, plus two proportional equations, one of which is for ozone. By making the equations dimensionless and making various assumptions, such as the emissions ratio of NO to NO2, the dimensionless quantities are solvable by hand. Knowing these, the equilibrium concentration of the five pollutant species can be obtained.

The disadvantages of this model are that it uses a simple advection scheme, eliminates dispersion and further simplifies an already simple chemical kinetics mechanism. Its advantage is that the various equations can be solved by hand without the use of computer.

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Spatial Resolution

Horizontal - single area cover of about 100 km2

Vertical - the height of the single layer box is a function of atmospheric stability. It is essentially the height of the mixed layer.

Temporal Resolution

One hour

Meteorology

A unidirectional wind is used to ventilate the reaction "box". The purpose of the wind is to limit the residence and hence reaction time of the precursors.

Chemistry

The ATDL model has used the Friedlander-Seinfeld chemistry (Friedlander, 1969) which consists of three reactions for NO2, NO and reactive hydrocarbons and two proportional relationships, one of which is for ozone calculations.

Input Data Requirements

Meteorological Variables - wind speed

Emissions Data - hourly emissions data for the box area for each of the species involved in the chemical reactions

Air Quality Data - none

Key Output

Predictions of ozone, NO, NO2 and reactive hydrocarbon levels for the study area.

APPLICABILITY OF THE HANNA ATDL PHOTOCHEMICAL MODEL TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

The Hanna ATDL model uses a simplification of the 1969 Friedlander-Seinfeld chemistry to predict ambient concentrations of NO2, NO and reactive hydrocarbons as a function of each species' source strength. Ozone is calculated as the ratio of the predicted NO2 to NO levels times a constant based on observed data. Thus to have valid ozone results, the NO2 and NO predictions must be accurate.

In one study (Hanna, July, 1973), the model was shown to predict NO and reactive hydrocarbon values reasonably well. However, the NO2 results showed little agreement with the observed levels. This is consistent with the discrepancy between estimated and observed ozone concentrations because of the dependency of the estimated ozone level on the estimated NO2/NO ratio.

Because the model (based on the Friedlander-Seinfeld) chemistry has not produced accurate NO2 and thus ozone predictions, it cannot be used at this time to address this issue even though the ATDL model has the capability to accept varying hydrocarbon and NOx emissions.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

The model has not performed well in predicting either NO2 or ozone levels, and thus should not be used for this purpose without further development and/or validation testing.

Control of Low-Level vs Elevated Emissions

The ATDL is a single-layer, well-mixed box model. Emissions are assumed to immediately disperse uniformly within the confines of the study area. Thus no distinction is made between low-level and elevated sources. The ATDL model is not applicable to this issue.

Selective Control of Hydrocarbon Compounds

A single hydrocarbon class is used for the photochemical simulations. The model is not applicable to this issue.

Long-Range Transport

The model is restricted to predictions within a stationary square area. It cannot be used to address this issue.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

The model accepts hourly aggregated NO, NO2 and reactive hydrocarbon emissions. It can address questions of temporal variations by asuming different emission rates for each calculation. Because the Hanna ADTL model is a well-mixed box model, the spatial variation of emissions cannot be evaluated.

ELSTAR

(ENVIRONMENTAL LAGRANGIAN SIMULATOR OF TRANSPORT AND ATMOSPHERIC REACTIONS)

MODEL FEATURES

Model Type

Lagrangian Trajectory

Historical Data

ELSTAR is the name of the photochemical trajectory model delivered to the Coordinating Research Council. A model similar to ELSTAR has been delivered to EPA who plans to release it in the near future (original release date March, 1979) [Lloyd, December, 1978]. This set of computer codes supersedes the DIFKIN model which was developed in 1973 (Martinez, 1973).

The DIFKIN version has been used in many applications, particularly for highway impact studies (Allen, 1976). ELSTAR has been applied to the St. Louis area (Lloyd, December, 1978).

Spatial Resolution

Horizontal - variable, user-specified

Vertical - the distance between the surface and stable layer can be divided into a number of equal height layers of any desired depth. Ten layers have been used.

Temporal Resolution

Hourly time steps for input and output.

Meteorology

ELSTAR uses a mass-consistent wind field along a trajectory defined by the flow of the wind and bounded in the vertical by the ground and mixing height. Within the wind field, vertical mixing between the layers is assumed to be due solely to turbulence.

Chemistry

45-step reaction mechanism

Five hydrocarbon classes: paraffins, olefins, aromatics, higher aldehydes and formaldehyde.

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Input Data Requirements

Meteorological Variables - wind speed and direction, temperature, humidity, diffusivity coefficients as a function of height, inversion height field, longitude and latitude and date.

Emissions Data - an hourly gridded emission inventory for the study area. Emissions of the following seven compounds must be input: NOx, CO, paraffins, olefins, aromatics, formaldehyde and higher aldehydes.

Air Quality Data - concentrations for all input species plus ozone at the start of the trajectory. Model verification requires concentrations of all input species and ozone along the trajectory path.

Key Outputs

Concentrations of ozone and other user-selected species along the trajectory path at hourly intervals for each vertical layer. One set of outputs is produced per trajectory.

Approximate Computer Requirements

A twelve-hour simulation requires 40 to 60 seconds of computer time on a CDC 7600 per trajectory. The number of trajectories required to fully characterize an area is a function of the complexity of the terrain and the heterogeneity of the spatial distribution of the emission sources in the study area. The observed pollutant concentration fields would indicate the spatial variability of the area and the number of trajectories necessary to fully define the study zone. In areas where a great number of trajectories are required, use of an Eulerian model might be more economical.

APPLICABILITY OF ELSTAR TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

ELSTAR has a photochemical simulation module which relates hydrocarbon and NOx emissions to resultant ozone concentrations. It can be used to address this issue. DIFKIN, the predecessor model, has been used to weigh the merits of varying degrees of hydrocarbon and/or NOx emission control on ozone formation (Allen, 1976).

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

ELSTAR can predict hourly NO2 and ozone values along the selected trajectory. It therefore can be used to evaluate the emission reduction necessary to meet both standards. These control strategies are often detrimental to the other pollutant. For the St. Louis study (see ref. Lloyd, et. al., 1978) the model's NO2 prediction capability was a major evaluation criterion.

Control of Low-Level vs Elevated Emission

ELSTAR distinguishes between low-level and elevated emission sources in its calculations. Emissions are dispersed into that vertical grid cell which corresponds to the effective plume rise of the individual source. Thus, ELSTAR is applicable to evaluating the effectiveness of control strategies aimed at either low level or elevated emission sources, or combinations of the two.

Selective Control of Hydrocarbon Compounds

ELSTAR can be used to address this issue because hydrocarbons are disaggregated into five classes before being input to the photochemistry module. Emissions of each class can be independently varied, simulating selective hydrocarbon control schemes, to study their effect on ozone formation.

Long-Range Transport

Because ELSTAR is a trajectory model, the effects of horizontal turbulence and shear forces in all three dimensions are assumed to be negligible. In other words, the air parcel is assumed to remain intact as it traverses along the trajectory. For short distances, this can be a valid assumption. However, as the travel time and distance become greater, the effect of horizontal shear becomes more pronounced. One way to reduce the effect of this force is to go to a coarser grid scale. This would have the effect of damping the peak concentration because the polluants would be averaged over a larger area. Another problem area is how a trajectory model would handle transport of pollutants in an inversion layer, which is an area of high wind shear.

Before ELSTAR can be used to address this issue, further field validation would be needed.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

ELSTAR can be used to evaluate control strategies based on this issue because the model retains the temporal and spatial characteristics of emissions in its calculation. However, these variations only affect the ozone results if the trajectories pass directly over the source(s) being altered.

TRACE

(TRAJECTORY ATMOSPHERIC CHEMISTRY AND EMISSIONS)

MODEL FEATURES

Model Type

Lagrangian trajectory

Historical Data

TRACE, released in November, 1977 (Drivas, March, 1977 and Drivas, November, 1977) is the latest version of the REM I (Wayne, 1973) and REM II (Drivas, February, 1977) trajectory models first developed in 1973. TRACE and its predecessors have been used in the preparation of many environmental impact reports for large point sources such as offshore oil terminals.

Spatial Resolution

Horizontal - variable, user-specified

Vertical - none, a single well-mixed layer is assumed

Temporal Resolution

One-hour intervals for input and output

Meteorology

A mass-consistent flow field defined in the vertical by the ground and the inversion base represent the trajectory of the air parcel.

Chemistry

Uses the EKMA chemistry (76-step reaction mechanism).

Three hydrocarbon classes: propylene, butane, and aldehydes.

Input Data Requirements

Meteorological Variables - wind speed and direction, temperature, humidity, inversion height and date.

Emissions Data - a gridded hourly emission inventory for all emissions disaggregated into NO, NO2 and the three hydrocarbon classes.

Air Quality Data - concentrations for all input species and ozone at the start of the trajectory. For model verification, concentrations of all input species and ozone along the trajectory path are needed.

Key Outputs

Tabulation of predicted ozone and user-selected species concentrations on an hourly basis along the trajectory. One set of outputs is produced per trajectory.

Approximate Computer Requirements

A 12-hour simulation of a single trajectory requires about 3 minutes of calculation time on an IBM 370/158.

APPLICABILITY OF TRACE TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

TRACE uses the EKMA chemistry module for photochemical simulations. This chemistry is suited to evaluating the ozone reduction due to decreases in hydrocarbon and/or NOx emissions; thus, TRACE is applicable to this issue.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

TRACE can be used to predict both the NO2 and ozone concentrations resulting from hydrocarbon and NOx emissions. Because of this, it can be used to evaluate the tradeoffs between reductions of hydrocarbon or NOx emissions necessary to achieving both standards.

Control of Low-Level vs Elevated Emission

TRACE is a single-layer trajectory model. It resembles a reaction chamber which is being blown along a path defined by the wind. Emissions entering the air parcel are assumed to become uniformly and instantaneously mixed. No distiction is made between low-level and elevated sources. Therefore the model cannot be used to address this issue.

Selective Control of Hydrocarbon Compounds

The TRACE chemical kinetic mechanism is the same as that used in the city-specific EKMA. It distinguishes three classes of hydrocarbons, butane, propylene, and aldehydes. Each can be varied to determine its effect on oxidant formation along a selected trajectory and for a given meteorological scenario, and selective hydrocarbon control schemes can be simulated.

Long-Range Transport

TRACE is a single-layer trajectory model based on the assumption that a single well-mixed column of air traveling along a trajectory will stay intact. In actuality, this column of air is acted upon in all three dimensions by wind shear and diffusion. This assumption, together with TRACE's inability to simulate transport in the inversion field because it is limited to a single layer, severely limits the model for addressing this issue.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

TRACE can be used to evaluate spatial and temporal variations in emissions along its trajectory path.

LIRAQ-2

(LIVERMORE REGIONAL AIR QUALITY MODEL, VERSION 2)

MODEL FEATURES

Model Type

Eulerian grid

Historical Data

LIRAQ-1, a nonphotochemical version, was published in 1972. This was supplemented in 1975 by a photochemical version called LIRAQ-2 (MacCracken, 1975, MacCracken, 1978, and Bass, 1977). The only difference in the two is that the latter has a photochemical simulation module. In 1977, the LIRAQ-2 version was updated to include sulfate chemistry simulation. Both LIRAQ-1 and 2 were used to develop the Air Quality Maintenance Plan (ABAG, 1977 and Duewer, 1978) and the 1979 Non-Attainment Area Plan for the San Francisco Bay Area. It is presently being applied to the St. Louis area.

Spatial Resolution

Horizontal - variable, user-specified. In previous applications, one to five kilometer square grids arranged in a 20 x 20 square array have been used. The largest areal coverage studied was 100 km x 100 km using a five kilometer grid.

Vertical - single layer from the surface to the top of the mixed layer with an imposed, fitted concentration profile.

Temporal Resolution

Variable time step, graphical output available at 30-minute intervals.

Meteorology

LIRAQ uses a mass-consistent flow field specifying depth of mixed layer, wind speed and direction for each grid cell; this field is interpolated for each hour from fields produced at three-hour intervals. An additional code, MASCON, is available to derive flow fields from hourly-averaged wind and mixing depth data.

Chemistry

48-step reaction mechanism
three hydrocarbon classes: alkanes, alkenes (olefins), aldehydes

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Input Data Requirements

Meteorological Variables - wind speed, direction, temperature, humidity, inversion height, topography, latitude, longitude, date.

Emissions Data - gridded hourly emissions inventory for area and point sources within the study area disaggregated into seven species: alkanes, alkenes, aldehydes, nitric oxide (NO), carbon monoxide (CO), sulfur dioxide (SO2) and particulates. The first four species are used in the photochemical simulation.

Air Quality Data - model operation requires ambient concentrations of all emitted species plus ozone at the boundaries all day and for the entire study area for the first hour simulated. Verification further requires a thorough sample of ozone, NO2 and other species concentrations in several cells for each hour of the prototype day being simulated.

Key Outputs

Tabular data provided for ozone and a variety of species. Concentration fields for all species calculated by LIRAQ can be output as isopleth maps.

Hour-by-hour plots of pollutant concentrations for oxidant, NO2, and each input species at user-specified grid locations.

Approximate Computer Requirements

A 24-hour simulation with a 20 x 20 x 1 grid requires 60 minutes of machine time and 1 million bytes on a CDC 7600.

APPLICABILITY OF LIRAQ-2 TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

Because LIRAQ-2 does have an algorithm to simulate the photochemical reactions between hydrocarbons and NOx to form ozone, it can be used to address this issue.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

LIRAQ is theoretically applicable to addressing the attainment of both an ozone and an NO2 standard because of its photochemistry module. It can evaluate the tradeoffs between an optimal ozone and an optimal NO2 control strategy to meet both standards.

However, before such a decision can be made with LIRAQ, some refinement of the NO2 predictions must be made. In previous experience with the model its simulation of NO2 levels on high ozone days (as opposed to high NO2 days) is generally not as good as the ozone simulation.

Control of Low-Level vs Elevated Emission

In its emission inventory, LIRAQ does require a separate file for low-level and elevated emission sources though it is basically a single-layer model. Elevated sources are assumed to affect only the vertical average concentration if below the inversion layer. The amount of the emissions used in the calculations are dependent on the height of the inversion base (Duewer, 1978). These sources are not included in the calculation of the vertical profile which is used to determine the ozone concentration within a cell. Therefore, LIRAQ is not applicable to this issue.

Selective Control of Hydrocarbon Compounds

The LIRAQ chemical kinetic mechanism distinguishes three classes of hydrocarbon source emissions. Variations in emissions of these three classes can be tested for their effect on ozone formation. LIRAQ's applicability to this issue is limited to the types of variations that can be simulated with the three hydrocarbon classes.

Long-Range Transport

LIRAQ could be modified to evaluate transport of pollutants into adjacent regions by increasing the grid size to large distances, e.g., ten km. However, if there is a significant possibility that the transport mechanism involves some vertical transport component rather than simple horizontal flow, or transport in the inversion layer which is subjected to significant wind shear (a simulation capability that LIRAQ lacks) then LIRAQ could not be applied.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

Since LIRAQ is a deterministic model which retains the spatial and temporal characteristics of emissions in its calculations, it is well-suited to evaluating the effects of variation of these parameters on ozone formation within the area covered by the grid.

SAI AIRSHED

MODEL FEATURES

Model Type

Eulerian grid

Historical

The SAI AIRSHED model has been in continuous development since the early 70's. In 1973, it was first used for a study of the Los Angeles area (Reynolds, 1973). Since that study many changes have been made to the model including a new photochemistry module. These modifications were all documented for the present version (Reynolds, 1978 and Reynolds, 1979). AIRSHED has been applied to many areas including Los Angeles, Denver, Sacramento, and St. Louis.

Spatial Resolution

Horizontal - variable, user-specified. AIRSHED has been run with 1 to 10 km square grids arranged rectangularly to cover the study area. The largest study area was Los Angeles with a grid of roughly 300 x 150 km.

Vertical - up to 10 vertical cells of these usually at least one is within the mixed layer and at least one is in the inversion.

Temporal Resolution

User-specified resolution of input and output.

Meteorology

Mass-consistent three-dimensional wind field including the depth of the mixed layer, wind shear between layers and cells and wind speed and direction in three dimensions for each grid cell for each layer. At present, one of the wind field input preparation algorithms is intended for use in areas where thermal, topographical and frictional effects on wind flow are not pronounced. Another code more applicable to a complicated terrain is now being evaluated; in addition, a straightforward inverse distance weighted interpolation scheme is also available.

Chemistry

31-step reaction mechanism

Four hydrocarbon classes: single-bonded carbon atoms, very reactive double-bonded carbon atoms, moderately reactive double-bonded atoms and carbonyl-bonded carbon atoms. These types

of bonds are characteristic of paraffins, olefins, aromatics and aldehydes, respectively.

Input Requirements

Meteorological Variables - wind speed and direction at the surface and for each vertical layer; inversion height field; insolation observations; temperature, pressure, relative humidity and topography: latitude and longitude and date.

Emissions Data - a gridded hourly emission inventory for all area and point sources located within the study area. Emission rates for the following species must be included for the photochemical simulation: NOx, CO, paraffins, olefins, aromatics and aldehydes.

Air Quality Data - model operation requires ambient concentrations of all emitted species plus ozone at the boundaries all day and for the entire study area for the first hour simulated. Verification further requires a thorough sample of ozone, NO2 and other species concentrations in several cells for each hour of the prototype day being simulated.

Key Outputs

Tabular concentrations of ozone and each input species at hourly intervals (option available through the developer for producing isopleth plots of each species).

Approximate Computer Requirements

A 14-hour simulation with a 25 x 25 x 4 grid requires 20 minutes of machine time and nearly 1 million bytes on a CDC 7600.

APPLICABILITY OF AIRSHED TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

With its photochemical simulation capabilities, AIRSHED can be used to assess the validity of control schemes aimed at reducing hydrocarbons and/or NOx to achieve the ozone standard. Therefore, AIRSHED is applicable to this issue. It was used in Denver to assess various HC/NOx control schemes (Anderson, 1977).

This issue has been specifically addressed in several studies: in the Los Angeles region, four schemes for controlling vehicular HC and/or NOx were evaluated; in Denver, various HC and/or NOx control schemes were examined; and various HC/NOx control schemes based on demographic changes for a number of areas were studied.

Assessing Attainment of the Ozone Standard for a Short-Term NO2 Standard

AIRSHED can predict NO2 levels in addition to ozone so that it can evaluate the control strategies necessary for achieving a short-term NO2 standard and an ozone standard. The model has been used to predict hourly NO2 levels in Los Angeles (Reynolds, 1973), Denver (Anderson, 1977) and St. Louis. The model performance for these NO2 predictions has generally been found to be somewhat poorer than for ozone. However, NO2 concentrations on these study days were generally relatively low. There is a need to further establish the model's NO2 performance characteristics.

Control of Low-Level vs Elevated Emissions

AIRSHED is applicable to this issue because it is a multi-layer model in the vertical, and it can distinguish between low-level and elevated emissions. Emissions are added to the layer corresponding to their total effective plume rise. If this height exceeds the top of the modeling region, the pollutants are excluded from subsequent AIRSHED calculations. For ground-level sources, emissions are added to the lowest layer. The model has been used to evaluate the impact of emissions from major elevated point sources on regional air quality.

Selective Control of Hydrocarbon Compounds

AIRSHED separates hydrocarbons into four classes according to the reactivity of the carbon bond. The distribution of the actual hydrocarbons can be changed to reflect control strategies. This would result in a change in each hydrocarbon category that contains the actual emissions. AIRSHED can be used to answer the question of hydrocarbon reactivity control.

Long-Range Transport

AIRSHED has been developed with enough generalities and includes treatment of wind shear and transport in the inversion layer so that it can theoretically be used to evaluate the transport of pollutants from one air basin into an adjacent region by expanding the grid size to ten km, for example. (The largest region to which the model has been applied is 150 to 300 km. on a side.) With the expanded scale, the adjacent region would become a part of the study area. Before this model or any model can be applied to a long-range transport analysis, it must be verified.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

Because AIRSHED is a deterministic Eulerian model, its emissions must be defined with spatial and temporal characteristics. Thus, it is well suited to studying the effects of varying the diurnal emission cycle and of varying the spatial distribution of precursors on ozone formation within the study area. AIRSHED has been used for this purpose in the Los Angeles (Anderson, 1977) and Denver (Reynolds, 1977) areas.

IMPACT

(INTEGRATED MODEL FOR PLUMES AND ATMOSPHERICS IN COMPLEX TERRAIN)

MODEL FEATURES

Model Type

Eulerian grid

Historical Data

IMPACT (Fabrick, 1977 and Ranzieri, 1979) was released in March 1977. It is an update of the DEPICT model (Sklarew, 1976). Since its release, the model has been used for a study in the Sacramento area (Amar, 1978).

Spatial Resolution

Horizontal - variable resolution, user-specified for each application

Vertical - 50 to 200 meters per layer. The number of layers is limited by computational requirements.

Temporal Resolution

One hour interval for input and output.

Meteorology

IMPACT uses a mass-consistent flow field specifying depth of mixed layer, wind speed and direction at the surface and for the vertical layer over each horizontal grid cell for each hour of simulation.

Chemistry

Two chemical kinetic mechanisms are provided as user options:

Mechanism # 1 - Five species including 1 hydrocarbon class (limited to 12-hour daytime simulation)

Mechanism # 2 - Fourteen species including four hydrocarbon classes: olefins, aromatics, paraffins, and aldehydes

Input Data Requirements

Meteorological Variables - wind speed and direction, topography, inversion height field, longitude and latitude, insolation, temperature, pressure, relative humidity, date.

Emissions Data - a gridded, hourly emission inventory for all area and point sources in the study zone. For the simpler chemical kinetic mechanism, the inventory should include three species: NO2, NO, and HC (reactive hydrocarbons). For the #2 chemistry, the following inputs should be provided: NO2, NO, olefins, aromatics, paraffins, aldehydes.

Air Quality Data - concentrations for all input species and ozone along the study area boundary and for as many grid cells as are available at the start of the simulation run should be provided. For model verification, these air quality data should be available for every hour of the simulation day.

Key Outputs

Two-dimensional array of hourly-average concentrations of ozone and other user-specified species for each vertical level at each prediction point.

Contour plot of species concentrations for each hour.

Approximate Computer Requirements

A 12-hour simulation of a 25 x 25 x 10 grid requires about 1 million bytes of memory and one hour of computation on an IBM 370/168.

APPLICABILITY OF IMPACT TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

The model IMPACT can be used to address this issue because it can simulate the HC/NOx relationship in ozone formation. The model has been applied to evaluate the effects of concurrent hydrocarbon and NOx emissions reductions.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

The model can be used to generate concurrent NO2 and ozone levels. Therefore, it can be used to address this topic.

Control of Low-Level vs Elevated Emissions

The model accepts both area and point sources. Area sources are considered to be low-level emissions while point sources are considered to be elevated. Several codes are available as options in IMPACT to determine total plume rise from these sources. There are no major differences among the options which are provided to make the model more general. The point source emissions are added to the vertical grid cell coinciding with the final plume height of the source. Thus, IMPACT is well-formulated to address this issue.

Selective Control of Hydrocarbon Compounds

The simpler chemical kinetic mechanism involves only a single hydrocarbon class and thus cannot be used to address this issue. The more complex chemical kinetic mechanism utilizes four classes of hydrocarbons (olefins, aromatics, paraffins and aldehydes) to represent non-methane hydrocarbon emissions. The quantity of each of these species can be varied to simulate the effects of selective hydrocarbon control schemes on ozone formation.

Long-Range Transport

IMPACT could theoretically be used to address long-range transport by modifying the wind generation module to verify its capability to transport pollutants in an inversion layer. However, as for all the models in this study, further field verification would be needed before IMPACT could be applied.

Effects of Spatial and Temporal Variation of Ozone Precursor Emissions

IMPACT is a deterministic grid-based model. Emissions must be fixed within the study area and a temporal distribution allotted to each. Thus, the model can be used to evalute this issue.

MADCAP (MODEL OF ADVECTION, DIFFUSION AND CHEMISTRY OF AIR POLLUTION)

MODEL FEATURES

Model Type

Eulerian grid

Historical Data

MADCAP was developed in 1978. The San Diego area is using the model in their non-attainment planning process (Sklarew, 1979).

Spatial Resolution

Horizontal - variable, user-specified. The largest area studied is a 37 x 51 grid of 2 km cells for the San Diego area.

Vertical - five layers divided at the following elevations: 50, 75, 125, 250 and 500 meters.

Temporal Resolution

One hour resolution of input and output.

Meteorology

MADCAP uses a mass-consistent three dimensional flow field specifying depth of mixed layer, wind speed and direction at the surface and for the vertical layer over each horizontal grid cell for each hour of simulation. This is the same wind field module as in IMPACT.

Chemistry

(Uses the LIRAQ-2 chemistry)

48-step reaction mechanism

Three hydrocarbon classes: alkanes, alkenes (olefins), aldehydes

Input Data Requirements

Meteorological Variables - wind speed and direction; inversion height field, insolation, temperature, pressure, relative humidity, topography, site location and date.

Emissions Data - a gridded hourly emission inventory of all area and point sources in the study region. Seven species must be included: alkanes, alkenes, aldehydes, nitric oxide, carbon monoxide, sulfur dioxide and particulates. (For hydrocarbon

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sources, MADCAP has a list of 17 source types and their relative hydrocarbon splits.) NOx is divided into NO and NO2 according to weighting factors for three source types.

Air Quality Data - concentrations for all input species and ozone at the boundaries of the study area and for as many grid cells as are available at the start of the simulation day are needed. For model verification these values should be available for every hour of the run.

Key Outputs

Tabular printouts of hourly ozone and other user-specified species concentrations at selected sites. Isopleth maps for oxidant and each desired species can also be generated at user option.

Hour-by-hour plots of pollutant concentrations for ozone and each input species at user-specified locations.

Approximate Computer Requirement

For an 11-hour simulation using a 37 x 51 x 5 grid of 2 km resolution in the horizontal, MADCAP requires about 1 hour of computation time on a Univac 1100/80. Core requirement is about 185,000 words of a 4 byte-memory (740,000 bytes). This cost does not include the emissions inventory and wind field generation subroutines whose output is fed into MADCAP.

APPLICABILITY OF MADCAP TO OZONE CONTROL STRATEGY ISSUES

Hydrocarbon vs NOx Control

MADCAP uses the LIRAQ-2 photochemical kinetic mechanism to simulate ozone production. This mechanism is capable of accepting varying HC and NOx emission levels and predicting the resultant ozone concentration. Thus, MADCAP can address this issue.

Assessing Attainment of the Ozone Standard and a Short-Term NO2 Standard

MADCAP can predict both ozone and NO2 concentrations so that it can be used to discern whether an optimal ozone reduction scheme is counterproductive to attaining an NO2 standard or vice-versa. Some further refinement might be needed before the model can be used for such an assessment because in the San Diego study, some problems in accuracy were encountered (Sklarew, 1979). It is conjectured that much of the error is due to the NOx emission split into NO and NO2.

Control of Low-Level vs Elevated Emissions

Five vertical layers are built into MADCAP. Emissions can be added into any of the layers. The bottom layer is comprised of low-level sources while point sources are added to that vertical layer corresponding to their total effective plume height. If this height exceeds the maximum study height of 500 m, the emissions are excluded from subsequent calculations. Thus the model does distinguish between sources of different height and can be used to address this issue.

Selective Control of Hydrocarbon Compounds

Hydrocarbons are divided into three categories, based on their reactivity: olefins, aliphatic aldehydes, and alkanes. Each of these hydrocarbon classes can be varied to study the effect of different emissions ratios on ozone formation. MADCAP can be applied to this issue.

Long-Range Transport

Before using MADCAP for long-range transport, two things need to be done: 1) the wind field module would need to be verified as to its capability to simulate pollutant transport in the inversion layer; and 2) the model needs to be verified with actual data (as do all the models in this report.)

Effects of Spatial and Temporal Variation of Ozone Precusor Emissions

Being a deterministic model, MADCAP retains spatial and temporal emission characteristics in its calculation. Thus, MADCAP can be used to address variations in these parameters.

RECOMMENDATIONS FOR FUTURE WORK

After undergoing several years of development and specialized applications, ozone models are increasingly being used to support air quality decision-making across the nation. A central role is envisioned for these models in the development of State Implementation Plan revisions for ozone. With this in mind, the immediate needs for further work consist of what is necessary to convert existing models from research tools to widely-disseminated, user-oriented, decision-making tools. These needs may be divided into two categories: (1) further performance evaluation and sensitivity analysis; and (2) improving user services.

FURTHER PERFORMANCE EVALUATION AND SENSITIVITY ANALYSIS

A number of unresolved questions regarding the performance of photochemical models can be identified. The most obvious is that for many of the control strategy issues posed in this report, no "track record" of model applications is available. The development of such track records is crucial so that model users interested in investigating one or more of these issues will have a base of experience by which data requirements, model applicability, experimental design and model performance may be judged.

The existing methodology by which model performance is evaluated involves the comparison of model-simulated ozone distributions to measured ozone distributions under a variety of prototypical meteorological conditions. Stated differently, the models' performance in response to varying meteorological conditions is compared with what is actually measured. Conversely, in long-range planning applications, such as will be required for the preparation of State Implementation Plan revisions, it is the models' performance in response to varying hydrocarbon and NOx emissions levels and distributions that is important. Demonstration of "good" performance under varying meterological conditions does not necessarily imply good performance under varying emissions conditions. Therefore, a different approach to model verification should be devised which would be responsive to this major area of model application.

A third recommendation related to performance evaluation is that a set of performance standards or guidelines should be developed to aid model users in assessing the adequacy of a model's performance in a given region before the model is used in a decision-making context. Currently, there is no objective measure to assess the adequacy of a model's performance in a given situation. Without a uniform set of performance standards it becomes the responsibility of each user to judge the acceptability of a model for any given application.

Finally, an important unknown at this time is the relationship between model performance and the quantity and quality of the meteorological, emissions, and air quality input data. Since resources for model

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applications are limited, potential model users will be concerned with the cost of input data collection and preparation. At the present time very little information is available on how the quantity and quality of input data for different variables affects model performance.

IMPROVING USER SERVICES

Since the number of potential photochemical model users is expected to increase substantially over the next few years, the demand for various services to users will increase. Such services may include:

- Periodic update and maintenance of model codes to include the most recent data (e.g., rate constants for chemical kinetics mechanisms)
- Code optimization for large, complex models to reduce their resource requirements
- Preparation of more detailed user-oriented handbooks on models to reduce the level of expertise required to use them
- Provision of low - or no-cost services to users for designing and troubleshooting model application projects.

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16. ABSTRACT

This document is an assessment of the applicability of a number of selected photochemical models to a variety of ozone control strategy issues. The issues include: hydrocarbon vs. NO_x control; applicability to NO_2 strategy assessment; low-level vs. elevated emissions; selective control of hydrocarbon compounds; long-range transport; and spatial and temporal variation of ozone precursor emissions. The specific models reviewed are as follows: linear rollback; EKMA; OZIPP; Hanna ATDL; ELSTAR; TRACE; LIRAQ; SAI Urban Airshed Model; IMPACT; and MADCAP. Data requirements, costs, and output produced by each model are also compared.

17. KEY WORDS AND DOCUMENT ANALYSIS

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